Dehydrocostus lactone

Other names: (3aS,6aR,9aR,9bS)-3,6,9-Trimethylenedecahydroazuleno[4,5-b]furan-2(9bH)-one
Inchi: InChI=1S/C15H18O2/c1-8-4-7-12-10(3)15(16)17-14(12)13-9(2)5-6-11(8)13/h11-14H,1-7H
InchiKey: NETSQGRTUNRXEO-UHFFFAOYSA-N
Formula: C15H18O2
SMILES: C=C1C(=O)OC2C1CCC(=C)C1CCC(=C)C12
Mol. weight [g/mol]: 230.30
CAS: 477-43-0

Physical Properties

Property code	Value	Unit	Source
gf	152.09	kJ/mol	Joback Method
hf	-196.49	kJ/mol	Joback Method
hfus	25.69	kJ/mol	Joback Method
hvap	58.34	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.017		Crippen Method
mcvol	184.170	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	2006.70		NIST Webbook
tb	667.48	K	Joback Method
tc	903.06	K	Joback Method
tf	430.14	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.26	J/mol×K	667.48	Joback Method
cpg	558.54	J/mol×K	706.74	Joback Method
cpg	577.44	J/mol×K	746.01	Joback Method
cpg	595.00	J/mol×K	785.27	Joback Method
cpg	611.26	J/mol×K	824.53	Joback Method
cpg	626.27	J/mol×K	863.80	Joback Method
cpg	640.05	J/mol×K	903.06	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C477430&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume